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Procedia Materials Science 3 (2014) 2065 – 2070

Procedia Materials Science

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20th European Conference on Fracture (ECF20)

Theoretical-numerical approaches to simulate fracture in polymeric materials

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Abstract

Fracture in structures is usually to be avoided or, if intended like for airbags or peel foils, it should occur along a predefined crack path. The integrity and usability of a part has to be ensured over the lifetime of the structure. In order to optimize a structure at the design stage, simulations allow to analyze and to predict the structural behavior for a development of the best layout. The contribution at hand presents appropriated material modeling strategies for polymers and introduces the so-called configurational force approach for inelasticity and finite strains as a method to analyze the energy release rate, the crack advancement and the crack growth direction. Certain numerical methods like cohesive elements, containing e.g. inelastic cohesive zone models and the node splitting approach combined with an r-adaptive discretization are shown as valuable simulation features.

Selection and peer-review under responsibility of the Norwegian University of Science and Technology (NTNU), Department of Structural Engineering

Keywords: polymers; finite element method; inelastic constitutive properties; crack growth

1. Introduction

Polymeric material exhibits complex constitutive features. Elastomers, for example, are characterized by large deformations and nonlinear elasticity. Moreover, rate-dependent viscoelastic properties as well as rate-independent behavior are found which have to be depicted by appropriate constitutive formulations. These inelastic properties combined with micro-damage and discrete fracture cause dissipation of mechanical energy. In consequence, heat is generated which might change the mechanical features. Thus, a coupled consideration of the thermal and the mechanical field is required, i.e. for the bulk material as well as the contact surfaces of heterogeneous solids or crack flanks within solids. In this case, thermomechanical interface descriptions can be used e.g. to predict the thermomechanical behavior of a solid with a designated failure layer. One of the main difficulties with respect to investigating fracturing is to realistically assess the failure sensitivity and failure behavior in structures even at the post-critical stage. In this contribution, the configurational force approach is used to obtain the energy release rate for inelastic material at finite strains and to predict crack propagation from an initial notch in a rubber sample.

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Selection and peer-review under responsibility of the Norwegian University of Science and Technology (NTNU), Department of Structural Engineering
doi:10.1016/j.mspro.2014.06.334

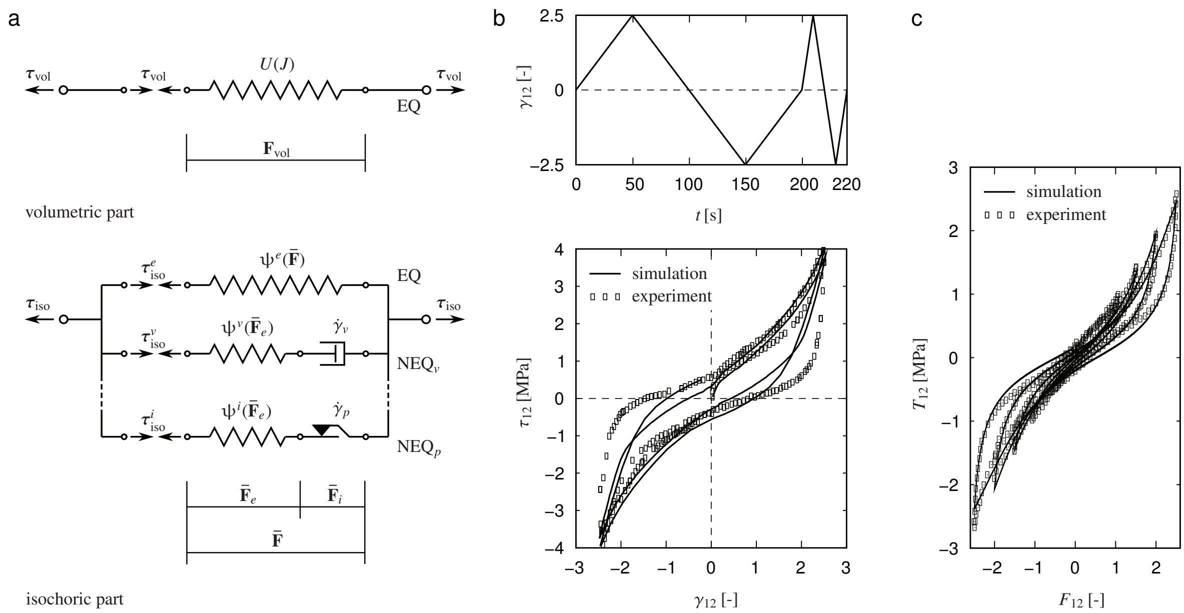

Fig. 1. Modeling of polymeric material: (a) rheology with strain energy functions $U(J)$, $\psi^e(\bar{\mathbf{F}})$, $\psi^v(\bar{\mathbf{F}}_e)$, $\psi^i(\bar{\mathbf{F}}_e)$ and deformation gradient $\mathbf{F} = \bar{\mathbf{F}}\,\mathbf{F}_{vol}$, $\mathbf{F}_{vol} = J^{1/3}\mathbf{1}$, $\bar{\mathbf{F}} = J^{-1/3}\,\mathbf{F} = \bar{\mathbf{F}}_e\,\bar{\mathbf{F}}_i$ as well as stress tensors $\boldsymbol{\tau}$; (b) cyclic simple shear tests, comparison of simulation results (EQ and NEQ$_v$) to experimental results from Amin et al. (2006); (c) cyclic simple shear tests, comparison of simulation results (EQ and NEQ$_p$) with experimental results from Besdo and Ihlemann (2003).

2. Material modeling

Polymers show a nonlinear ground state elasticity (equilibrium response – EQ) and more or less pronounced inelastic features, as described e.g. in Grellmann et al. (2013). To represent rate-dependent viscoelastic properties of polymers (viscous non-equilibrium response – NEQ$_v$), a nonlinear spring/dashpot combination with a strain-dependent evolution law for the rate of inelastic dashpot deformations $\dot{\gamma}_v$ has been implemented in the finite element framework by Dal and Kaliske (2009). The rheology of the material model is depicted in Fig. 1 (a). Rate-independent plastic behavior without a distinctive yield surface (plastic non-equilibrium response – NEQ$_p$) has been captured by a nonlinear spring/friction element in series, where the rate of inelastic deformation $\dot{\gamma}_p$ of the friction element is governed by an endochronic evolution equation with an internal time measure, see Netzker et al. (2010). The comparable, modular structure of the implementation allows to set up generalized material models describing combinations of rate-dependent and rate-independent non-equilibrium behavior of the polymers. In Fig. 1 (b), the modeling of rate-dependent viscoelastic properties (NEQ$_v$) has been compared to experimental data whereas in Fig. 1 (c), rate-independent plastic behavior has been successfully simulated using the endochronic plasticity formulation (NEQ$_p$). The hysteresis loops recorded during the cyclic tests show the dissipative nature of the inelastic effects. The dissipation of mechanical energy and a consecutive heating of the compounds have been included in the simulation approach by a fully coupled finite element formulation with a simultaneous solution scheme, see e.g. Behnke et al. (2011).

3. Fracture mechanical approaches

3.1. Configurational force approach

The configurational force approach allows to consider inelastic effects at large strains (Näser et al. (2007)) as well as temperature- and inertia-induced contributions to crack propagation. In a post-processing step, configurational forces are computed to assess fracture sensitivities and to obtain suitable criteria for crack propagation within numerical simulations. In Fig. 2, configurational force contributions, computed at a crack tip of an elasto-plastic plate, are

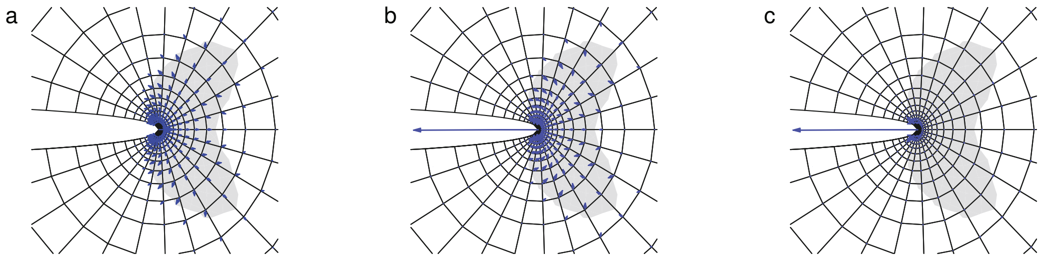

Fig. 2. Crack tip in a plate made of elasto-plastic material, see Kaliske et al. (2012): (a) material volume nodal forces stemming from inelastic deformations; (b) material nodal forces as driving forces on the crack tip and the process zone; (c) crack driving forces as the sum of material volume nodal forces (a) and material nodal forces (b).

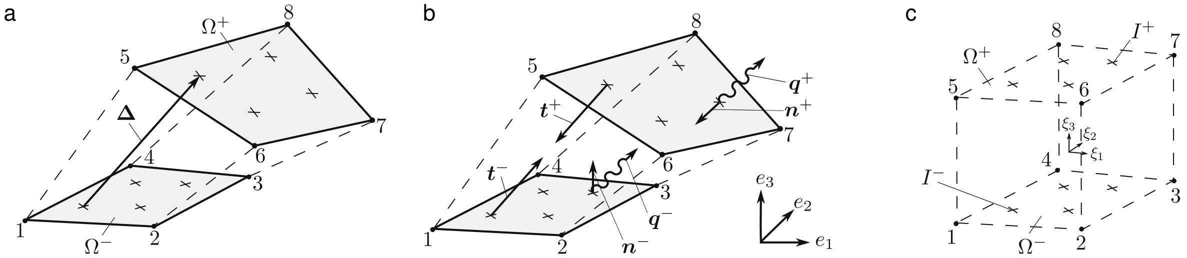

Fig. 3. Linear interface element: (a) separation $\boldsymbol{\Delta}$; (b) current normals $\boldsymbol{n}^+$, $\boldsymbol{n}^-$, current tractions $\boldsymbol{t}^+$, $\boldsymbol{t}^-$ and spatial heat fluxes $\boldsymbol{q}^+$, $\boldsymbol{q}^-$; (c) isoparametric space with local coordinates $\boldsymbol{\xi}$ and integration points I^+, I^-.

depicted. An inelastic process zone around the crack tip is clearly visible which induces configurational volume forces. The configurational volume forces, shown in Fig. 2 (b), will reduce the pure crack driving force at the crack tip plotted in Fig. 2 (c). In Netzker et al. (2013), the energy release rate and the configurational force approach are evaluated for inelastic polymeric material and the material's sensitivity to stable crack propagation is investigated.

3.2. Thermomechanical cohesive elements

Different cohesive zone models and interface element formulations have been developed, see e.g. the recent ones proposed by Bosch et al. (2007) and Bosch et al. (2008) for a large deformation description as well as an extension to thermomechanics by Özdemir et al. (2010). In contrast to existing mechanical and thermomechanical interface element formulations, a thermodynamically consistent finite deformation framework for modeling interfacial effects as well as discrete cracks is presented in Fleischhauer et al. (2013).

In terms of an interface between two subbodies B_i and B_k forming the body B, the boundaries $\partial B_i \supset \Omega$ and $\partial B_k \supset \Omega$ are piecewise identical along the connective interface $\Omega \subset B$. The opening displacement between two points $(+) \in \Omega$ and $(-) \in \Omega$ can be described by the opening vector $\boldsymbol{\Delta} = \boldsymbol{x}^+ - \boldsymbol{x}^-$, where $\boldsymbol{x}^+ \in B_i$ and $\boldsymbol{x}^- \in B_k$. The related points are initially connected having the same coordinates $\boldsymbol{X}^+ \in B_i$, $\boldsymbol{X}^- \in B_k$ at Ω^+_{ref} and Ω^-_{ref}. Both points start to separate as soon as the bonding between them is smaller than its connective forces. Furthermore, the temperature jump $[\![\theta]\!] = \theta^+ - \theta^-$ at the points (+) and (−) is introduced. The contribution of an interface element to the discretized balance of linear momentum for B reads

$$-\boldsymbol{f}^E_{ifc} = -\int_{\Omega^+_E} \boldsymbol{N}^T_{\Omega^+} \boldsymbol{t}^+ d\Omega^+ - \int_{\Omega^-_E} \boldsymbol{N}^T_{\Omega^-} \boldsymbol{t}^- d\Omega^- \,. \tag{1}$$

According to the isoparametric concept of the finite element method, e.g. linear ansatz functions $\boldsymbol{N}_{\Omega^+}$ and $\boldsymbol{N}_{\Omega^-}$ for the shape of the interface element, containing local coordinates $\boldsymbol{\xi}$ (compare Fig. 3) can be used. The interface element contribution to the discretized transient heat conduction equation for the temperature evolution in B, reads

$$\boldsymbol{h}^E_{ifc} = \int\limits_{\Omega^+_E} \boldsymbol{N}^T_{\theta\Omega^+}(\boldsymbol{q}^+ \cdot \boldsymbol{n}^+ - w^+)d\Omega^+ + \int\limits_{\Omega^-_E} \boldsymbol{N}^T_{\theta\Omega^-}(\boldsymbol{q}^- \cdot \boldsymbol{n}^- - w^-)d\Omega^- \;, \tag{2}$$

where linear ansatz functions $\boldsymbol{N}_{\theta\Omega^+}$ and $\boldsymbol{N}_{\theta\Omega^-}$ are used. The thermal conduction energies $h^+ = (\boldsymbol{q}^+ \cdot \boldsymbol{n}^+)$ and $h^- = (\boldsymbol{q}^- \cdot \boldsymbol{n}^-)$, as well as the power terms $w^+ = w^+_{ext} - w^+_{int}$ and $w^- = w^-_{ext} - w^-_{int}$ describe the rate of energy of the surfaces Ω^+ and Ω^-, since they are originated in the heat flux and the power terms of the bonds between the opening flanks.

Modeling of time-dependent cohesive fracture is addressed in Geißler and Kaliske (2010) via a cohesive element formulation that still distinguishes between normal and tangential directions at the crack surface. In contrast to that, the model rheology presented in Zreid et al. (2013) consists of a parallel acting spring and spring/dashpot combinations for finite separations of the crack faces. The stiffness of the springs is described using an exponential traction-separation law. The total separation vector $\boldsymbol{\Delta}$ is divided into elastic $\boldsymbol{\Delta}^e$ and viscous $\boldsymbol{\Delta}^v$ parts. The total tractions are the sum of the elastic and viscous tractions. The time-independent and viscous tractions read

$$\mathbf{T}^e = \frac{\phi}{\delta^2}\exp\left(-\frac{||\boldsymbol{\Delta}||}{\delta}\right)\exp\left(\frac{-\vartheta}{\theta_b}\right)\boldsymbol{\Delta} \quad \text{and} \quad \mathbf{T}^v = \beta\frac{\phi}{\delta^2}\exp\left(-\frac{||\boldsymbol{\Delta}||}{\delta}\right)\exp\left(\frac{-\vartheta}{\theta_b}\right)(\boldsymbol{\Delta} - \boldsymbol{\Delta}^v) \;, \tag{3}$$

where β is a material parameter describing the relation between the elastic and the viscous tractions. ϕ is a material parameter representing the work required for complete separation and δ is the characteristic opening length. θ_b is a material parameter which determines the sensitivity of the cohesive zone stiffness with respect to the temperature change. The cohesive law used here is characterized by a single work of separation, which means that the energy dissipation is independent of the mode-mixture. This assumption is valid in case of large deformation and where the main mechanism of interface bridging is the formation of fibrils, which is the case for polymeric materials. The evolution law for the internal variable $\boldsymbol{\Delta}^v$ and the heat conduction law are taken as

$$\dot{\boldsymbol{\Delta}}^v = \frac{\delta}{\eta}\mathbf{T}^v \quad \text{and} \quad \mathbf{Q}\cdot\mathbf{N} = -(1-d)\,k_s\,[\![\theta]\!] \;, \tag{4}$$

where η is a constant viscosity. Here, the heat conduction law is a phenomenological description assuming that the transfer of heat occurs along the connective bonds and is caused by the difference in temperature $[\![\theta]\!]$ between the two interface surfaces. k_s is the interface heat conductivity and $d = \frac{\Delta_{max}}{\Delta_{cr}}$ is a damage parameter that quantifies the reduction of conductivity due to separation. Δ_{max} is the norm of the maximum separation reached during the loading history and Δ_{cr} is the separation value at which the conduction stops completely. The described model is used to simulate the peel process of a thin polymeric film. The experimental results, which are taken from Geißler et al. (2007), are performed on sealed Polyethylene/Polybutene-1 (PE) films. The peeling test geometry, the finite element discretization and the model parameters are given in Zreid et al. (2013). The results of the simulations and the comparison to experimental data are shown in Fig. 4. The viscoelastic features of the model are applied to capture the measured peel force at different loading rates $\dot{u}$ using the same set of material parameters.

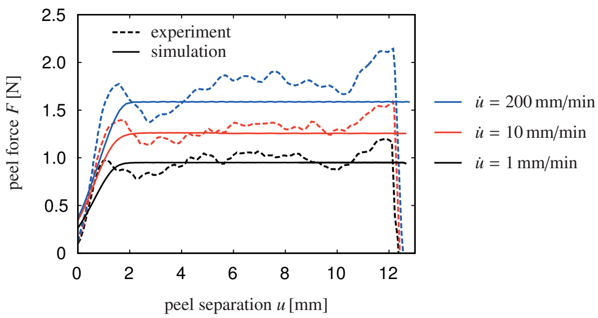

Fig. 4. Comparison of numerically and experimentally obtained force-separation curves for different loading speeds.

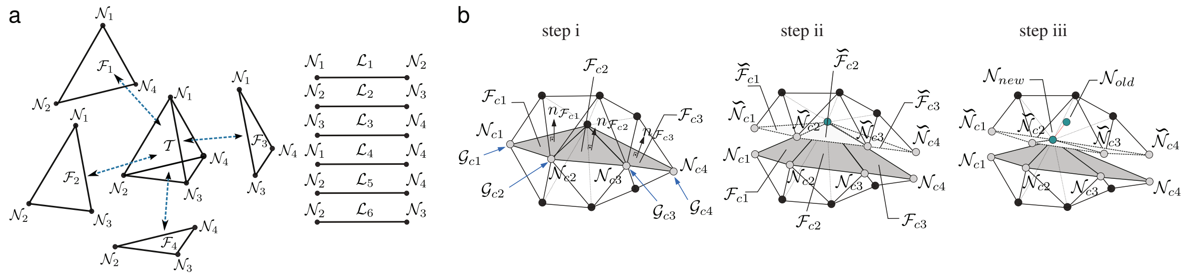

Fig. 5. Node duplication method: (a) data structure of objects; tetrahedral element $\mathcal{T}$, face $\mathcal{F}$ and line $\mathcal{L}$; (b) schematic description of the algorithm used to simulate the failure of element faces.

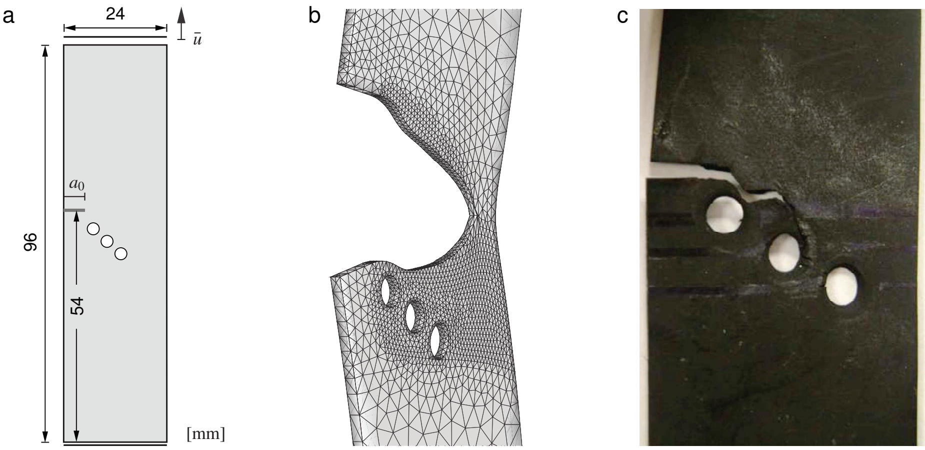

Fig. 6. Comparison of the numerical computation to the experimental data for the failure mechanism of an asymmetric single edge notched specimen under tension: (a) boundary conditions and geometry; (b) final deformed mesh; (c) result of experimental study from Ozelo et al. (2012).

3.3. Arbitrary crack growth

A node duplication method has been adapted to investigate fracture phenomena in hyperelastic polymeric material. In order to use the node duplication method with r-adaptation strategies, a specific data structure is always required to simulate the failure of element faces. Similar to the model proposed by Miehe and Gürses (2007), in this contribution (see Özenç et al. (2014) for further details), a tetrahedral element $\mathcal{T}$ is introduced. The schematic view of the data structure is illustrated in Fig. 5 (a). Initially, the data structure remains unchanged unless the criteria reach a critical value. In general, an advancement of the crack requires three steps. First, the standard connectivity information and numerical solution of the finite elements is stored. Second, a new data structure from the last topology has to be formed. Third, history data belonging to internal variables and displacement fields need to be mapped for the numerical solution of the next time step in case of inelastic material features. After this procedure, an additional regulation is necessary in order to ensure the numerical stability in nonlinear analyses. In Fig. 5 (b), the adaptive algorithm for doubling the critical faces and the critical nodes is sketched. Here, $\mathcal{G}_c$ is a configurational force resultant at node $\mathcal{N}_c$ which gives the fracture criterion and the crack propagation direction. After having found the crack propagation direction, the critical face $\mathcal{F}_c$ needs to be determined. When this is accomplished, the crack tip nodes can be duplicated by their mutual ones $\tilde{\mathcal{N}}_c$. After the last step, the new crack surface is aligned to the required direction by moving the node. The described algorithm is used to simulate an asymmetric single edge notched specimen with three holes at tension. Experimental results have been published by Ozelo et al. (2012). In Fig. 6 (a), the geometric setup of the specimen is given as well as its boundary conditions. For the simulation, 8427 tetrahedral elements are used. One of the main advantages of the proposed method is not just its robustness but also that the model successfully describes the crack trajectories for quite rough meshes. Therefore, the computation cost of the process is moderate. In the numerical study, the material is modeled using the 8-chain model (or Arruda and Boyce model), implemented within a linear displacement based element. In Fig 6 (b), the simulated crack trajectories are shown whereas Fig. 6 (c) depicts the crack trajectories from the experimental study. The comparison of the simulation results to the experimental results shows that the crack path does agree with the experimental one, i.e. the model captures also kinking cracks.

4. Conclusions

In this contribution, strategies for the representation of polymeric material and its thermo-mechanical behavior with respect to deformation and fracture are discussed. Each subproblem (material modeling, representation of discrete fracture and incorporation of crack driving criteria) is very complex and has to be considered in a combined simulation concept to obtain realistic and reliable design tools. The setup of such advanced but still efficient coupled simulation concepts is still object of current research.

Acknowledgments

The authors acknowledge the support by the Deutsche Forschungsgemeinschaft (DFG) under grant KA 1163/16.

References

Amin, A., Lion, A., Sekita, S., Okui, Y., 2006. Nonlinear dependence of viscosity in modeling the rate-dependent response of natural and high damping rubbers in compression and shear: Experimental identification and numerical verification. International Journal of Plasticity 22, 1610–1657.

Behnke, R., Dal, H., Kaliske, M., 2011. An extended tube model for thermo-viscoelasticity of rubberlike materials: Theory and numerical implementation, in: Jerrams, S., Murphy, N. (Eds.), Constitutive Models for Rubber VII, Taylor & Francis Group, London. pp. 87–92.

Besdo, D., Ihlemann, J., 2003. A phenomenological constitutive model for rubberlike materials and its numerical applications. International Journal of Plasticity 19, 1019–1036.

Van den Bosch, M.J., Schreurs, P.J.G. and Geers, M.G.D., 2007. A cohesive zone model with large displacement formulation accounting for interfacial fibrilation. European Journal of Mechanics A/Solids 26, 1–19.

Van den Bosch, M.J., Schreurs, P.J.G. and Geers, M.G.D., 2008. On the development of a 3D cohesive zone element in the presence of large deformations. Computational Mechanics 42, 171–180.

Dal, H., Kaliske, M., 2009. Bergström-Boyce model for nonlinear finite rubber viscoelasticity: Theoretical aspects and algorithmic treatment for the FE method. Computational Mechanics 44, 809–823.

Fleischhauer, R., Behnke, R. and Kaliske, M., 2013. A thermomechanical interface element formulation for finite deformations. Computational Mechanics 52, 1039–1058.

Geißler, G., Kaliske, M., Nase, M., Grellmann, W., 2007. Peel process simulation of sealed polymeric film computational modelling of experimental results. Engineering Computations 24, 586–607.

Geißler, G. and Kaliske, M., 2010. Time-dependent cohesive zone modelling for discrete fracture simulation. Engineering Fracture Mechanics 77, 153–169.

Grellmann, W., Heinrich, G., Kaliske, M., Klüppel, M., Schneider, K., Vilgis, T. (Eds.), 2013. Fracture Mechanics and Statistical Mechanics of Reinforced Elastomeric Blends. Volume 70 of *Lecture Notes in Applied and Computational Mechanics*. Springer-Verlag Berlin.

Kaliske, M., Dal, H., Fleischhauer, R., Jenkel, C., Netzker, C., 2012. Characterization of fracture processes by continuum and discrete modelling. Computational Mechanics 50, 303–320.

Miehe, C. and Gürses, E., 2007. A robust algorithm for configurational-force-driven brittle crack propagation with r-adaptive mesh alignment. International Journal for Numerical Methods in Engineering 72, 127–155.

Näser, B., Kaliske, M., Müller, R., 2007. Material forces for inelastic models at large strains: Application to fracture mechanics. Computational Mechanics 40, 1005–1013.

Netzker, C., Dal, H., Kaliske, M., 2010. An endochronic plasticity formulation for filled rubber. International Journal of Solids and Structures 47, 2371–2379.

Netzker, C., Horst, T., Reincke, K., Behnke, R., Kaliske, M., Heinrich, G., Grellmann, W., 2013. Analysis of stable crack propagation in filled rubber based on a global energy balance. International Journal of Fracture 181, 13–23.

Özdemir, I., Brekelmans, W.A.M.. and Geers, M.G.D., 2010. A thermo-mechanical cohesive zone model. Computational Mechanics 46, 735–745.

Ozelo, R.R.M., Sollero, P. and Costa, A.L.A., 2012. An alternative technique to evaluate crack propagation path in hyperelastic materials. Tire Science and Technology 40, 42–58.

Özenç, K., Kaliske, M., Lin, G. and Bashyam, G. 2014. Evaluation of Energy Contributions in Elasto-Plastic Fracture: a Review of the Configurational Force Approach. Engineering Fracture Mechanics 115, 137–153.

Zreid, I., Fleischhauer, R. and Kaliske, M. 2013. A thermomechanically coupled viscoelastic cohesive zone model at large deformation. International Journal of Solids and Structures 50, 4279–4291.